Ethylene oxide

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 11.9 °C

Global applicability domain: Inside

Local applicability domain index: 6.61e-01

Confidence level: 7.50e-01

Nearest Neighbors from the Training Set

Image not found
Ethylene oxide
Measured: 10.6
Predicted: 11.9

Image not found
Acetaldehyde
Measured: 20.1
Predicted: 23.9

Image not found
Cyclopropane
Measured: -32.8
Predicted: -24.5

Image not found
Peroxide, dimethyl
Measured: 14.0
Predicted: 18.4

Image not found
Chloromethyl methyl ether
Measured: 59.5
Predicted: 48.3